CJ 06/30/23
TW 06/30/23
JS 8/18/23

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98 [redacted]

Case #: P-13-0858	**DCN:**
SAT Date: 9/6/2013	**SAT Chair:** J. Kwiat

Submitter: Canon USA Inc

Chemical Name:

[redacted]

CAS RN: [redacted]

Structure

[redacted]

Molecular Formula: [redacted]		
Molecular Wt. [redacted]	**WT%<500:**	**WT%<1000:**
MP: [redacted]	**BP:** [redacted]	**Eq. Wt:**
H2O Sol (g/L): [redacted]	**V.P.** [redacted]	
Max. Prod. Volume (kg/yr): [redacted]	**Physical State:**	Yellowish solid

USE:

[redacted]

Related Case Numbers	Case Role	Related Case Numbers	Case Role
[redacted]	Incomplete: do not use		

Focus Date: 9/16/13 Results: DROP

SAT Report

PMN Number: **P-13-0858**
SAT Date: **9/6/2013**
Print Date: **9/6/2013**

Related cases:

Health related cases: [redacted]
Ecotox related cases: Same as [redacted]. Analogs: [redacted]

Concern levels:

Type of Concern:	Health	Eco	Comments
Level of Concern:	1-2	3	

Persistence	Bioaccum	Toxicity	Comments
1	1	1	

Exposure Based Review:

Health: No
Ecotox: No

Routes of exposure:

Health: Dermal Drinking Water Inhalation
Ecotox: All releases to water
Fate: ;

Keywords:

Keywords:
NEURO
LIVER
UNCERT SYSTOX
AQUATOX-A,C

Summary of Assessment:

Fate:

Fate Summary: P-13-0858

FATE:
Solid with MP = [redacted] C (M)
log Kow = [redacted] (M)
S = [redacted] mg/L at 25 C (M)
VP = [redacted] torr at 25 C (M)

BP = [redacted] C (M)
H = 8.09E+3 (E)
log Koc = [redacted] (M), 3.75 (E)
log Fish BCF = 3.14 (E)
log Fish BAF = 1.96 (E)
POTW removal (%) = 50-90 via sorption and biodeg; OECD 301B(Mod Sturm CO2 ev): 9%/28d NRB; OECD 302C(Modified Miti Test): 40.8%/28d (BOD), 65.3% (HPLC analysis); OECD 301(Closed Btl): 81%/28d; OECD not stated(Standard Closed Btl Test): 24%/28d; OECD not stated(Slightly Modified Closed Btl Test): 52-61%/28d.
Time for complete ultimate aerobic biodeg = wk
Sorption to soils/sediments = moderate
Volatilization half-life from a standard river = 2 hrs
Volatilization half-life from a standard lake = 8 da
Atmospheric Oxidation Half-life = 5.2 hr via OH radical
PBT Potential: P1B1
*CEB FATE: Migration to ground water = moderate

Health:

Health Summary: Absorption of the neat material is nil all routes, while absorption for the material in solution is poor all routes, based on physical/chemical properties. There are concerns for neurotoxicity and liver toxicity, as well as uncertain concern for systemic toxicity to the blood and endocrine system, based on submitted test data.

Test Data: Submitted with the PMN (same data set submitted with [redacted]

Negative in Salmonella with and without activation;
Negative in E. coli with and without activation;
Negative for chromosome aberrations in human lymphocytes with and without activation;
Rat acute (15D) oral (gavage) toxicity LD50 2000 mg/kg;
Rat acute (15D) dermal LD50 2000 mg/kg;
No eye irritation in rabbits;
No skin irritation in rabbits;
No skin sensitization in guinea pigs using the Magnusson-Kligman assay;
Rat 28-day oral NOEL 150 mg/kg, with signs of liver toxicity and neurotoxicity at 1000 mg/kg, and blood and endocrine system changes, not clearly related to dosing, in females at 1000 mg/kg

Ecotox:

Test Organism	Test Type	Test End Point	Predicted	Measured	Comments
fish	**96-h**	**LC50**	*	*	measured data submitted with [redacted]
daphnid	**48-h**	**LC50**	*	*	
green algal	**96-h**	**EC50**	0.179	*	

fish	_	**chronic value**	0.018		
daphnid	_	**chronic value**	0.185		
algal	_	**chronic value**	0.14	0.01	
Sewage Sludge	**3-h**	**EC50**	_		
Sewage Sludge	_	**Chronic Value**	_		

Ecotox Values Comments: Predictions are based on SARs for esters; SAR chemical class = ester; MW[redacted]; log Kow = [redacted] (M), 6.1 (ClogP); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; DW hardness < 150.0 mg/L as CaCO3; and DW TOC <2.0 mg/L;

Factors	Values	Comments
Assessment Factor	10	
Concentration of Concern (ppb)	1	
SARs	Esters	
SAR Class	Esters	
Ecotox Category	Esters	

Ecotox Factors Comments:

SAT Chair: J. Kwiat

GTOX Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer
S		nsh

		with activation	without activation	Positive Strains
Salmonella Assay:		N	N	
Chromosomal Aberration	CHO:			
	CHL:	N	N	
	V79:			
E.coli Reverse Mutation:		N	N	
	Route:			
Mouse Micronucleus Assay:				
Rat Hepatocytes Unscheduled DNA Synthesis:				

Other GTOX Results

Comments

ECOTOX: X

Fate: Ready Biodegradation (OECD TG 301B), p.337; Estimation of Adsorption Coefficient (OECD TG 121), p. 367.

WS/Log P: [redacted] g/L @ 19.5 +/- 1.0 deg C (M, p. 298); LogP = [redacted] @ 24.5 +/- 0.5 deg C (M, p.314).

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer	Study#:
S		nsh	1

Study Type	Species	Sex	Route
Acute Toxicity	Rat	MF	Gavage

Test Substance Description

Yellow white solid. Purity: +/- 95%. Vehicle: Propylene Glycol

Test Condition

Study duration: 15 days; Strain: Wistar; Wt/Life stage: 185 - 249 g (females), 295 - 430 g (males)/~ 8 weeks; No. Groups/No. Per Group: 2/3; Controls: NS; Dose Level: 2000 mg/kg bw; Test Conditions (Dose regimen): OECD TG 423. Animals received single dose of the test substance on day 1. Macroscopic examination was performed after terminal sacrifice on day 15.

RESULTS:

No mortality occurred and no clinical signs were noted. Animals experienced normal body weight gain and no abnormalities were found during the macroscopic examination of the animals. The oral LD50 exceeded 2000 mg/kg bw.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer	Study#:
S		nsh	2

Study Type	Species	Sex	Route
Acute Toxicity	Rat	MF	Dermal

Test Substance Description

Light yellowish solid. Purity: > 95%. Vehicle: Propylene glycol.

Test Condition

Study duration: 15 days; Strain: Wistar; Wt/Life stage: 183 - 250 g (females), 263 - 367 g(males)/~ 8 weeks; No. Groups/No. Per Group: 1/10 (5M & 5F); Controls: NS; Dose Level: 2000 mg/kg bw; Test Conditions (Dose regimen): OECD TG 402. Single dose of the test substance was administered on day 1 for 24 hours. Macroscopic examination was performed after terminal sacrifice on day 15.

RESULTS:

No mortality occurred. Clinical signs of toxicity included lethargy, hunched/flat posture and/or chromodacryorrhoea (most animals between days 1&6); diarrhoea and ptosis (some males on days 1&2); erythema (focal, maculate or general), scales, and/or scabs (treated skin of most animals). Animals experienced normal body weight gain. Enlargement of the mandibular lymph nodes (uni- or bilateral) was noted in two males and two females. No further abnormalities were found during the macroscopic examination of the animals. The dermal LD50 exceeded 2000 mg/kg bw.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer	Study#:
S		nsh	3

Study Type	Species	Sex	Route
Eye Irritation	Rabbit	M	Eyes

Test Substance Description

Yellowish solid. Purity: +/-95%.

Test Condition

Study duration: 72 hours; Strain: New Zealand White; Wt/Life stage: 1.0 - 3.5 kg /~ 6 weeks; No. Groups/No. Per Group: 1/3; Controls: NS; Dose Level: 0.1 ml; Test Conditions (Dose regimen): OECD TG 405. Single doses of the test substance were instiled into one eye of each animal. Observations were made at 1, 24, 48 and 72 hours after instillation.

RESULTS:

Instillation of the test substance resulted in irritation of the conjunctivae, reflected as redness, chemosis and discharge. The irritation had completely resolved within 24 hours in one animal and within 72 hours in the other animals. The test substance did not cause staining of the (peri) ocular tissues, but remnants of the test substance were present in the eyes of all animals on day 1. There was no evidence of ocular corrosion.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer	Study#:
S		nsh	4

Study Type	Species	Sex	Route
Dermal Irritation	Rabbit	M	Dermal

Test Substance Description

Yellowish solid. Purity: +/-95%.

Test Condition

Study duration: 72 hours; Strain: New Zealand White; Wt/Life stage: 1.0 - 3.5 kg/~ 6 weeks; No. Groups/No. Per Group: 1/3; Controls: NS; Dose Level: 0.5 g; Test Conditions (Dose regimen): OECD TG 404. Test substance was applied onto the clipped skin of the animals for 4-hours under semi-occlusive conditions. Observations were made 1, 24, 48 and 72 hours after exposure.

RESULTS:

There was no skin irritation or evidence of a corrosive effect.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer	Study#:
S		nsh	5

Study Type	Species	Sex	Route
Dermal Sensitization	Guinea pig	F	Dermal

Test Substance Description

Yellowish solid. Purity: +/- 95%. Vehicle: DMSO in corn oil.

Test Condition

Study duration: 24 days; Strain: Dunkin Hartley; Wt/Life stage: 305 - 536 g/~ 4 weeks; No. Groups/No. Per Group: 1/10; Controls: 1/5; Test Concentrations: 2%, 5% (main study); Test Conditions (Dose regimen): OECD TG 406. Animals were intradermally injected with a 2% concentration and epidermally exposed to a 5% concentration of the test substance. Control animals were similarly treated, but with vehicle alone (10% DMSO in corn oil). Two weeks after the epidermal application, all animals were challenged with a 2% test substance concentration and the vehicle.

RESULTS:

No mortality occurred and no symptoms of systemic toxicity were observed in the study animals. There was no evidence that the test substance caused skin hypersensitivity in the guinea pig since no responses were observed in the experimental and control animals during the challenge phase. Results indicate a sensitization rate of 0%.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer	Study#:
S		nsh	6

Study Type	Species	Sex	Route
Repeated Dose Toxicity	Rat	MF	Gavage

Test Substance Description

Light yellowish solid. Purity: > 95%. Vehicle: Propylene glycol

Test Condition

Study duration: 28 days; Strain: Wistar; Wt/Life stage: 209 - 409 g (males), 171 - 268 g (females)/NS; No. Groups/No. Per Group: 3/10 (each group contained 5M & 5F); Controls: propylene glycol, 1/10 (5M & 5F); Dose Levels: 50, 150, 1000 mg/kg/d; Test Conditions (Dose regimen): OECD TG 407. The test or control substance was administered to groups of rats for 28 days. The following parameters were evaluated: clinical signs daily; functional observation tests; body weight and food consumption weekly; clinical pathology and macroscopy at termination; organ weights and histopathology on a selection of tissues.

RESULTS:

No treatment-related findings were noted at 50 mg/kg/d. Females displayed increased individual motor activity recordings at 150 mg/kg/d. Signs observed at 1000 mg/kg/d included increased individual motor activity recordings (both males & females); and slightly low weight gain (males & females). Deviations in clinical biochemistry parameters observed in females dosed at 1000 mg/kg/d included increase alanine aminotransferase activity; increased alkaline phosphatase activity; increased urea levels in individual females; increased glucose level in one female; slightly increased inorganic phosphate level; and lower total protein level. Overall the relationship of these signs to the treatment with the test substance was considered to be uncertain. The NOAEL was 150 mg/kg/day.

GTOX Report

PMN No.	CAS No.	Recvd:	OECD	
P-13-0858	[redacted]	8/29/2013	Completed	ID: Rec# 7: 990

S/A Name of Analog

S

Reviewer

AA

		with activation	without activation	Positive Strains
Salmonella Assay:		N	N	
Chromosomal Aberration	CHO:			
	CHL:			
	V79:			
E.coli Reverse Mutation:		N	N	
	Route:			
Mouse Micronucleus Assay:				
Rat Hepatocytes Unscheduled DNA Synthesis:				

Other GTOX Results

No clastogenic effects were observed in human lymphocytes in an in vitro chromosome aberration test in the absence and presence of metabolic activation.

Comments

ECOTOX: X

Fate: Biodegradability Studies (Attachs. # 17, 9, & 12)
Inherent Biodegradability Study (Attach. # 17, support submission)

WS/Log P: WS: [redacted] g/L @ 20C, M (PMN pg. 13, Attach. #15)
LogP: [redacted] M (PMN pg. 13, Attach. # 16), [redacted] (Attach. # 4)

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
P-13-0858	[redacted]	8/29/2013	Completed	ID: Rec# 7: 990

S/A	Name of Analog	Reviewer	Study#:
S		AA	1222

Study Type	Species	Sex	Route
Acute Toxicity	Rat	MF	Gavage

Test Substance Description

Purity: +/- 95%; State: Yellow-white solid; Carrier: Propylene glycol.

Test Condition

Study duration: 15 days; Strain: Wistar; Wt/Life stage: 295-314 g males, 185-197 g females/~8 weeks old; No. Groups/No. Per Group: 2/3; Controls: NS; Dose Level: 2000 mg/kg-bw; Test Conditions (Dose regimen): OECD 423 acute oral toxicity- Substance was given to first group of 3 animals and upon observation of no severe effects, the second group was dosed in the same manner. The animals were then observed for systemic toxicity during the study period.

RESULTS:

No mortalities occurred and no clinical signs were noted. Body weights of the test animals were considered to be within a normal acceptable range. No abnormalities were observed at macroscopic post mortem examination of the animals. Based upon these results, the acute oral LD50 was greater than 2000 mg/kg-bw in rats.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
P-13-0858	[redacted]	8/29/2013	Completed	ID: Rec# 7: 990

S/A	Name of Analog	Reviewer	Study#:
S		AA	1223

Study Type	Species	Sex	Route
Acute Toxicity	Rat	MF	Dermal

Test Substance Description

Purity: >95%; State: Light yellowish solid; Carrier: Propylene glycol.

Test Condition

Study duration: 15 days; Strain: Wistar; Wt/Life stage: 263-294 g males, 183-203 g females/~8 weeks old; No. Groups/No. Per Group: 1/10 (5/sex); Controls: NS; Dose Level: 2000 mg/kg-bw; Test Conditions (Dose regimen): OECD 402 acute dermal toxicity-Substance was applied to clipped, intact skin for 24 hours with a semi-occlusive bandage. Following this exposure period, the dressing was removed and the site was rinsed. The animals were then observed for systemic toxicity during the study period.

RESULTS:

No mortalities occurred. Clinical signs included lethargy, hunched/flat posture and/or chromodacryorrhoea in the majority of animals between days 1 and 6. In addition, diarrhoea and ptosis were seen in some males on days 1 or 2. Also, erythema (focal, maculate or general), scales, and/or scabs were noted on the treated skin area of most animals during the observation period. Body weight changes were considered to be within a normal range. Macroscopic findings included enlargement of the mandibular lymph nodes (uni or bilateral) in two males and two females. No further abnormalities were noted. Based upon these results, the acute dermal LD50 was greater than 2000 mg/kg-bw in rats.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
P-13-0858	[redacted]	8/29/2013	Completed	ID: Rec# 7: 990

S/A	Name of Analog	Reviewer	Study#:
S		AA	1224

Study Type	Species	Sex	Route
Eye Irritation	Rabbit	M	Eyes

Test Substance Description

Purity: +/- 95%; State: Yellowish solid.

Test Condition

Study duration: 72 hours; Strain: New Zealand White; Wt/Life stage: 1475-1726 g/7-9 weeks old; No. Groups/No. Per Group: 1/3; Controls: Untreated eye; Dose Level: 0.1 mL; Test Conditions (Dose regimen): OECD 405 acute eye irritation/corrosion-Substance was placed into the conjunctival sac of the treated eye of three animals. Following instillation, observations were made at 1, 24, 48, and 72 hours. Immediately after the 24 hour observation, a solution of 2% fluorescein in water was instilled into both eyes of each animal to quantitatively determine corneal epithelial damage. Any bright green stained area, indicating epithelial damage, was estimated as a percentage of the total corneal area.

RESULTS:

No mortalities occurred and no systemic toxicity was observed. Irritation of the conjunctivae, which was seen as redness, chemosis, and discharge were noted in one animal for 24 hours and in two animals for 72 hours. Mean eye irritation scores (24-72 hours) for the three test animals were 0 for corneal opacity, iris, and chemosis, and 0.7 (two animals) and 0.0 for redness. No iridial irritation or corneal opacity was observed. Treatment of the eyes with 2% fluorescein 24 hours after test substance instillation revealed no corneal epithelial damage in any of the animals. No evidence of ocular corrosion or staining of (peri) ocular tissues by the test substance was observed. Remnants of the test substance were present in the eyes of all animals on day 1.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
P-13-0858	[redacted]	8/29/2013	Completed	ID: Rec# 7: 990

S/A	Name of Analog	Reviewer	Study#:
S		AA	1225

Study Type	Species	Sex	Route
Dermal Irritation	Rabbit	M	Dermal

Test Substance Description

Purity: +/- 95%; State: Yellowish solid; Carrier: Milli-U water.

Test Condition

Study duration: 76 hours; Strain: New Zealand White; Wt/Life stage: 1620-1683 g/7-9 weeks old; No. Groups/No. Per Group: 1/3; Controls: untreated skin; Dose Level: 0.5 grams; Test Conditions (Dose regimen): OECD 404 acute dermal irritation/corrosion-Substance was applied to clipped, intact skin for 4 hours with a semi-occlusive bandage. Following this exposure period, the dressing was removed and the site was rinsed and assessed at 1, 24, 48 and 72 hours.

RESULTS:

No mortalities occurred and no signs of systemic toxicity were observed. No evidence of a corrosive effect on the skin was noted, and no staining of the treated skin was observed. The mean value irritation scores (mean 24-72 hours) for erythema and oedema were 0 for all of the three animals tested.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
P-13-0858	[redacted]	8/29/2013	Completed	ID: Rec# 7: 990

S/A	Name of Analog	Reviewer	Study#:
S		AA	1226

Study Type	Species	Sex	Route
Dermal Sensitization	Guinea pig	F	Dermal

Test Substance Description

Purity: +/- 95%; State: Yellowish solid; Carroer: DMSO in corn oil.

Test Condition

Study duration: 24 days; Strain: Dunkin Hartley; Wt/Life stage: 305-382 g/~4 weeks old; No. Groups/No. Per Group: 1/10; Controls: 1/5; OECD 406 Skin Sensitization described by Magnusson and Kligman- Test guinea pigs were first injected with the test substance (0.1 mL) at three, prepared skin sites- cranial (1:1 w/w emulsified Freund's complete adjuvant with water for injection), midline (2% test item concentration in corn oil), and the caudal (1:1 w/w test item in emulsified Freund's complete adjuvant and a 4% test concentration). On Day 8, a dermal patch covered with 0.5 mL of test substance at 5% in corn oil was applied to the injection sites under occlusive conditions for 48 hours, and then removed for assessment. At both induction phases of the study, control animals were treated similarly but with the test item replaced by vehicle alone. On Day 21, test and control animals were exposed to a challenge patch consisting of 2% test substance concentration and 10% vehicle concentration (0.1 mL each) at the same injection sites for 24 hours. Test sites were assessed 24 and 48 hours after removal of the dressing.

RESULTS:

No mortalities or symptoms of systemic toxicity were observed. For the intradermal injection sites, erythema was noted in both the test and control animals at the cranial (scores 2 and 3), midline (scores 1 and 2), and caudal sites (scores 1 and 2). For the epidermal exposure sites, the erythema scores for the test and control animals were 0-1 and the oedema scores were all 0. No skin reactions were noted after the challenge exposure in the experimental and control groups. Body weights and body weight gain were considered to be within a normal range.

Toxicology Report

PMN No.	CAS No.	Recvd:	OECD	
[redacted]	[redacted]	11/6/2007	Completed	ID: Rec# 4: 938

S/A	Name of Analog	Reviewer	Study#:
S		nsh	6

Study Type	Species	Sex	Route
Repeated Dose Toxicity	Rat	MF	Gavage

Test Substance Description

Light yellowish solid. Purity: > 95%. Vehicle: Propylene glycol

Test Condition

Study duration: 28 days; Strain: Wistar; Wt/Life stage: 209 - 409 g (males), 171 - 268 g (females)/NS; No. Groups/No. Per Group: 3/10 (each group contained 5M & 5F); Controls: propylene glycol, 1/10 (5M & 5F); Dose Levels: 50, 150, 1000 mg/kg/d; Test Conditions (Dose regimen): OECD TG 407. The test or control substance was administered to groups of rats for 28 days. The following parameters were evaluated: clinical signs daily; functional observation tests; body weight and food consumption weekly; clinical pathology and macroscopy at termination; organ weights and histopathology on a selection of tissues.

RESULTS:

No treatment-related findings were noted at 50 mg/kg/d. Females displayed increased individual motor activity recordings at 150 mg/kg/d. Signs observed at 1000 mg/kg/d included increased individual motor activity recordings (both males & females); and slightly low weight gain (males & females). Deviations in clinical biochemistry parameters observed in females dosed at 1000 mg/kg/d included increase alanine aminotransferase activity; increased alkaline phosphatase activity; increased urea levels in individual females; increased glucose level in one female; slightly increased inorganic phosphate level; and lower total protein level. Overall the relationship of these signs to the treatment with the test substance was considered to be uncertain. The NOAEL was 150 mg/kg/day.

NCSAB SAT REPORT		CBI? (Y/N):
PMN: P-13-0858	CAS RN: [redacted]	
Chemical Name: [redacted]		Production Volume: [redacted]

Structure:

[redacted]

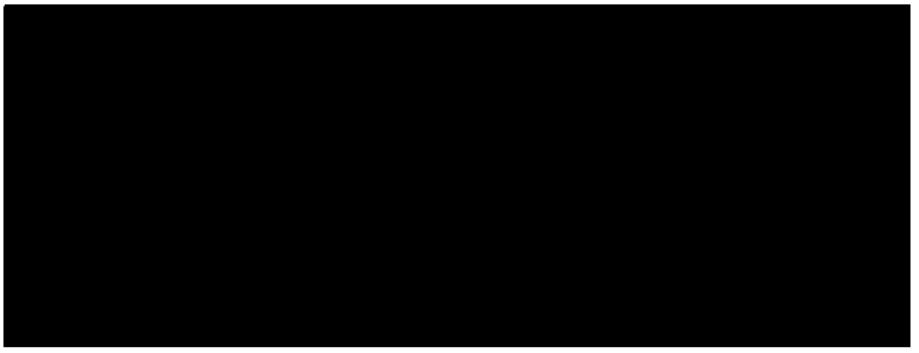
Use:

[redacted]

Formula: [redacted]	Eq Wt:	
Mol Weight: [redacted]	Wt%<500:	Wt%<1000
MP: [redacted]	BP: [redacted]	VP:
H2O Sol (g/L): [redacted]	Physical State: Yellowish solid	Log P:

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	*	*	Measured data submitted w/ [redacted]
Daphnid 48-h	*	*	
Algal 96-h	0.179	*	
Fish ChV	0.016		
Daphnid ChV	0.185		
Algal ChV	0.140	0.01	
BCF			

CHEMICAL CLASS:	SAR: Esters				
ECOTOX CONCERN	(H)	M	L	CONCERN CONCENTRATION	1 ppb
DATE 9-5-13				ASSESSOR: K. Moran	



ECOSAR Version 1.11 Results Page

SMILES : [redacted]
CHEM :
CAS Num:
ChemID1:
MOL FOR: [redacted]
MOL WT : 386.45
Log Kow: [redacted] (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: [redacted] (deg C, User Entered for Wat Sol estimate)
Melt Pt: (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: [redacted] (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: [redacted] (EPISuite Kowwin v1.68 Estimate)
Wat Sol: [redacted] (mg/L, EPISuite WSKowwin v1.43 Estimate)

Available Measured Data from ECOSAR Training Set

No Data Available

ECOSAR v1.1 Class-specific Estimations

Esters

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Esters	Fish	96-hr	LC50	0.505 *
Esters	Daphnid	48-hr	LC50	0.727 *
Esters	Green Algae	96-hr	EC50	0.179
Esters	Fish		ChV	0.018
Esters	Daphnid		ChV	0.185
Esters	Green Algae		ChV	0.140
Esters	Fish (SW)	96-hr	LC50	0.623 *
Esters	Mysid	96-hr	LC50	0.112
Esters	Fish (SW)		ChV	0.166
Esters	Mysid (SW)		ChV	0.007
Esters	Earthworm	14-day	LC50	391.606 *
Neutral Organic SAR (Baseline Toxicity)	Fish	96-hr	LC50	0.258 *
	Daphnid	48-hr	LC50	0.201 *

: Green Algae	96-hr	EC50	0.557 *
: Fish		ChV	0.037
: Daphnid		ChV	0.047
: Green Algae		ChV	0.296 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Esters:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE 9/6/13

ATTENDEES	SIGNATURE
CHEMISTRY	
___ Paul Bickart	
___ Diana Darling	
___ Greg Fritz	
✓ Kathy Schechter	Kathy Schechter
___ Richard Fehir	
___ Justin Roberts	
___ Jasbir Sarna	Jasbir Sarna
___ Rich Engler	
___ _____	
ENVIRONMENTAL FATE	
___ Bob Boethling	
___ Wen-Hsiung Lee	
___ Laurence Libelo	
___ David Lynch	
___ Andy Mamantov	
HEALTH	
___ Katherine Anitole	
✓ David Lai	V. Lai
✓ Viktor Morozov	
___ Jim Murphy	
___ Doritza P-Rodriguez	
___ Lemuel Russell	
___ Ronald Ward	
___ Yin Tak Woo	
___ _____	
ENVIRONMENTAL EFFECTS	
___ Gordon Cash	
___ Jeff Gallagher	
___ Maggie Johnson	
✓ Kendra Moran	
___ Sara Pollack	
SAT CHAIR/OTHER	
___ Rebecca Jones	
✓ Leonard Keifer	
✓ Jim Kwiat	
___ _____	